AD-A200 104 FIREBIRD 3 (HELLFIRE 7): A COMPUTER PROGRAM FOR CALCULATING THE POSITIONS..(U) UKAEA RISLEY NUCLEAR POWER DEVELOPMENT LABS (ENGLAND) I F FERGUSON ET AL. 1/1

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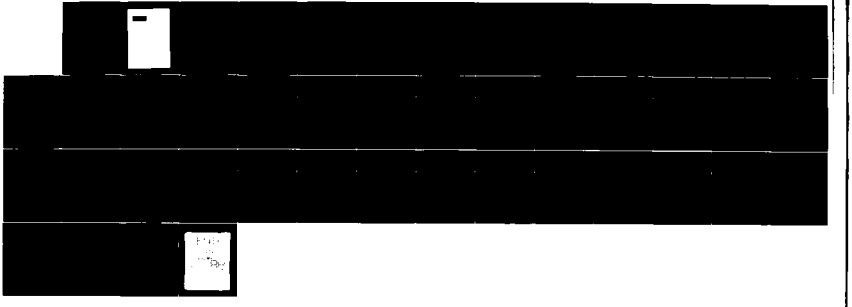

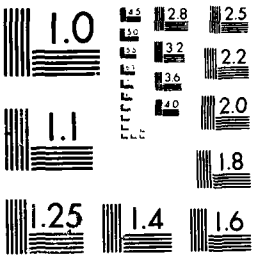

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FIREBIRD3 (HELLFIRE7)

A computer program for calculating the positions of reflections on X-ray powder diffraction records, interplanar angles, crystallographic densities and assigning indices to X-ray powder diffraction records

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SUMMARY

The program input consists of a definition of the unit cell, e.g. its space group, and dimensions; and the X-ray wavelengths used. From these data the program lists the positions of all the crystallographically possible X-ray Bragg reflections up to a maximum of 1000. If required, interplanar angles and crystal densities can be calculated. The program can vary the given unit cell dimensions and compare the resultant Bragg reflection positions with experimentally observed values, thereby acting as a guide for the assignment of Miller indices to X-ray powder patterns.

FIREBIRD3 is written in FORTRAN 77 for use on an ICL 3980 computer, and represents part of the HELLFIRE suite of computer programs.

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1. INTRODUCTION

In X-ray powder diffraction it is frequently necessary to predict the positions of the Bragg reflections which correspond to a given crystallographic unit cell. This is a trivial problem when the position of only a single Bragg reflection of known Miller indices is considered; while using a computer it is relatively simple to compute the position of all the possible Bragg reflections which correspond to a given unit cell (provided the computer store is big enough). However, it is not so easy to restrict the calculation to reflections which are crystallographically distinct, i.e. making due allowance for the symmetry properties of the Laue group to which the unit cell belongs, and moreover to exclude those reflections which are not allowed by the general space group symmetry of the unit cell considered. FIREBIRD3 has been written to do all these things and to execute calculations which relate to crystal densities and interplanar angles. Moreover, the program can vary a given set of lattice parameters over a pre-determined range and since it can also compare the calculated positions of Bragg reflections with those actually observed it can be used as a means to index X-ray powder diffraction patterns. The program can also produce blocks of Miller indices in a form suitable for transcription as input to the program FIREFLY[1] and in this sense should be considered as complementary to it.

FIREBIRD represents one of a series of programs developed at the UKAEA Northern Research Laboratories (Springfields) (SL) and at UKAEA, Risley.[2-4] Various programs have been developed elsewhere along these lines[5-12] but FIREBIRD3 is believed to represent the most satisfactory program at the present time.

FIREBIRD3 is one of a suite of programs developed at SL for the solution and interpretation of X-ray powder diffraction records,[1,13,14,15] and as such it also carries the designation HELLFIRE7. A complete list of the programs in the HELLFIRE suite is given in Appendix 8.

2. EQUATIONS SOLVED

Only standard crystallographic equations have been used. They are summarised here, but given in full in Appendix 1. The unit cell volume, V, is calculated from the lattice parameters (a, b, c, α, β and γ) of the crystallographic unit cell using the general formula for a triclinic unit cell.[16] The reciprocal lattice parameters are derived from the lattice parameters given by standard formulae.[16] The number of lattice points, n, within the limiting (Ewald) sphere is given by:

$$n = 32\pi V/3\lambda^3$$

where λ is the first X-ray wave-length considered.[17] The 'FLINT CODES'[18] which will be described later, is a set of numbers which specifies the general conditions limiting the possible reflections for a particular space group. The Bragg angle, θ, has been calculated using the formula appropriate to each crystal system.[19] The interplanar spacing, d(Å), is given from the Bragg equation

$$\lambda = 2d \sin\theta$$

where the order of the reflection has been ignored, since it is conventional to incorporate it within the Miller indices h, k and ℓ which describe a reflecting plane. The program never refers to the hexagonal Miller index i, which equals - (h+k), while it refers to the rhombohedral Miller indices as

h, k and ℓ rather than p, q and r. The program uses 'NSYS codes' to define the various Laue-symmetry groups. These codes, given in Appendix 2, were developed for the program FIREFLY.[1] They are used to derive the multiplicity of each reflection output and to define the non-equivalent arrangements of each Miller index. Interplanar angles relative to one or more given crystallographic reference planes are calculated using the general formulae for a triclinic unit cell.[16] The Nelson-Riley function referred to in certain outputs is given by the expression:

$$\frac{1}{2}\left(\frac{\cos^2\theta}{\sin\theta} + \frac{\cos^2\theta}{\theta}\right),$$

it is used in certain crystallographic extrapolation procedures.[19]

The program calculates the theoretical ('crystal') density, ρ, from the volume, V, of the unit cell, the molecular weight of its contents, M, and the Avogadro number, A, using the relation

$$\rho = M/AV$$

3. GENERAL AND SPECIFIC FEATURES

FIREBIRD3 uses the standard methods of data input applicable to FORTRAN 77; the detailed form of the data input is described later. The program operates on the equations referred to above. Thus, for a given set of unit cell dimensions, FIREBIRD calculates and outputs the unit cell volume, reciprocal lattice parameters, and the number of reciprocal lattice points corresponding to the first wavelength considered within the limiting (Ewald) sphere, (although the program makes no further use of the latter information). Then, provided it is given data which enable it to determine the molecular weight of the contents of the unit cell, it infers the crystallographic density.

The main role of the program is, however, to compute a list of the Bragg reflections, subject to certain constraints, for all possible Miller indices which can be produced by a given crystallographic unit cell, using X-ray (or electron) powder diffraction techniques. It does this by calculating $\sin^2\theta$ from the equation appropriate to the crystal system and/or setting, and/or lattice of the unit cell and the appropriate wavelength being considered.[16,19]

Various X-ray wavelengths, Cu $K\alpha_1$, Cu $K\alpha_2$, Cu $K\alpha$ (weighted mean), Cu $K\beta$, Cr $K\alpha_1$, Cr $K\alpha_2$, Cr $K\alpha$ (weighted mean), Fe $K\alpha_1$, Fe $K\alpha_2$, Fe $K\alpha$ (weighted mean), Co $K\alpha_1$, Co $K\alpha_2$, Co $K\alpha$ (weighted mean), Mo $K\alpha_1$, Mo $K\alpha_2$, Ag $K\alpha_1$, and Ag $K\alpha_2$ are stored within the program and referred to by codes in the data input. All this information, which is detailed in Appendix 3, has been taken or derived from Henry, Lipson and Wooster.[19] Since these wavelength values are subject to revision in the literature the preset values can be overwritten, as required, in the data input.

Provision is made for the program to make systematic variations in the lattice parameters given, so altering the predicted reflection positions. When these data are output alongside data which refer to observed reflection positions, it becomes possible, in principle, to assign Miller indices to any given set of observations. However, as the symmetry of the unit cell decreases, the computer time required rapidly becomes unreasonable. In the program's calculations, the crystal system is either derived directly from the Laue group input in coded form, or inferred from the space group.

The next section describes in some detail how the Miller indices are derived for each crystal system; while a further section explains how the general conditions which govern the allowed reflections from a particular space group are operated.

The number of reflections listed is limited to a maximum of 1000, or some other lower predetermined limit, or up to a preset Bragg angle. The reflections are output in order of increasing angle irrespective of the wavelength, which is referred to in each case by a numerical code.

Two statements appear at the end of each example. The first: THE NEXT HLK TO BE CONSIDERED WAS ... indicates the nex highest value of either h, k or ℓ beyond that considered in the output as ..uld have been expected according to the logic applicable to the crystal system being considered. The second statement THERE WERE ... HKL COMBINATIONS AVAILABLE ... indicates the number of valid sets of Miller indices for a particular example between 0 and 90°θ irrespective of those actually output.

3.1 THE CONDITIONS WHICH DETERMINE THE GENERATION OF h, k AND ℓ VALUES FOR EACH LAUE GROUP

The crystal system is either derived from the Laue group, input in coded form, or inferred from the space group, subject to the fact that the program is so written that the Laue group given overrides the space group. It will, moreover, be seen from the input specification, that various details of the space group or Laue group can be suppresssed in the data output.

In the cubic system, the maxium possible value of the Miller index, h, is first inferred, on the basis that $\sin^2\theta$ cannot exceed unity, or a value coresponding to the preset value of θ; it is a value which k and ℓ cannot exceed. Every wavelength is considered in this calculation. All possible positive arrangements of h, k and ℓ are then computed subject to the conditions that for the Laue group m3m, $h \geq k \geq \ell$; while for the Laue group m3, the m3m list is further extended by the interchange of h and k, i.e. k can exceed h.

In the tetragonal crystal system maximum values of h and ℓ are deduced as above. For the Laue group 4/mmm, all possible positive non-identical arrangements of h, k and ℓ are next inferred, subject to the overriding condition that k cannot exceed h. The tetragonal Laue group 4/m is treated as for 4/mmm except that k can become negative, unless it equals h.

For the orthorhombic system, Laue group mmm, each maximum value of h, k and ℓ is first inferred. The program then evaluates all different possible positive arrangements of h, k and ℓ.

For the hexagonal crystal system maximum values of h and ℓ are inferred as above. For the Laue group 6/mmm all possible positive non-identical arrangements of h, k and ℓ are then inferred subject to the overriding restriction that k cannot exceed h. However, for the Laue group 6/m k can additionally exceed h except for hOℓ when Ohℓ is not considered. When the trigonal Laue group 3 is considered as hexagonal it is treated as for Laue group 6/m above except that ℓ can also take negative values, i.e. hkℓ, khℓ, hkℓ and khℓ are all considered. Similarly when the Laue group $\bar{3}$m is treated as hexagonal it is evaluated as for $\bar{3}$ except that for hhℓ, hhℓ is not considered and for hkO, khO is not considered.

For the monoclinic crystal system, Laue group 2/m, second setting (the International Union of Crystallography preferred setting), the maximum values of h, k and ℓ are computed; the mixed index term (see Appendix 1) is ignored and each maximum value is arbitrarily tripled to allow for this. All possible positive non-identical arrangements of k and ℓ are then considered with all possible positive and negative values of h, except that when ℓ is zero h cannot be negative. The first setting of the monoclinic crystal system is treated similarly but k, instead of h, can become negative, except when h is zero. (If for the first setting $a = a$, $b = b$, $c = c$, $\gamma = \gamma$, then if the second setting is applied to the same crystal structure $a' = a$, $b' = c$, $c' = b$, $\beta = (180° - \gamma)$.

In the trigonal crystal system considered with a rhombohedral lattice and for the $\bar{3}m$ Laue group, nested loops are applied wherein h is increased, followed by k and then ℓ such that these values take only positive values and ℓ does not exceed k, and k does not exceed h. All possible values of h, k and ℓ are considered until either 1000 arrangements have been found which, allowing for subsequent tests, can be output, or 1000 arrangements have been considered, or the data input have imposed some other limit. In this way the $(h^2 + k^2 + \ell^2)$ term is found for the standard rhombohedral formula, see Appendix 1. The $(hk + k\ell + h\ell)$ term is next derived as follows: the values of h, k and ℓ already found are first considered as positive, each hk, kℓ and hℓ term is then allowed separately to become negative so that, in all, four values are found for the $(hk + k\ell + h\ell)$ term. However only different values of this term are considered further for each set of values of h, k and ℓ, i.e. $4\bar{3}2$ does not exclude $5\bar{2}0$. For the $\bar{3}$ Laue group treated as rhombohedral the same considerations apply except that for hkℓ, hℓk must also be output.

For the triclinic crystal system, Laue group $\bar{1}$, nested loops are applied in which h is increased, followed by k, followed by ℓ. Initially h, k and ℓ are all treated as positive and $\ell \geq k \geq h$. Next all combinations of each of these hkℓ arrangement are considered in which h, k and ℓ are independently either positive or negative, thus there are 72 possible arrangements based on 321. These computations stop when ten thousand sets of Miller indices have been considered, unless either a thousand values of θ have been output, or some other limit has been introduced in the data input.

3.2 THE GENERAL CONDITIONS LIMITING THE POSSIBLE REFLECTIONS FROM A SPACE GROUP - THE FLINT CODES

At this stage the program has calculated the angular position of all the Bragg reflections corresponding to a particular crystal system within certain limits. However, considerable numbers of reflections may be forbidden by the general symmetry of a particular space group e.g. for α-alumina only eighty reflections are actually allowed by the trigonal space group 167 whereas in terms of the crystal system alone 270 reflections would be predicted. For this reason nine digits, the FLINT codes, have been derived which summarise the reflections allowed by a particular space group. These codes are input to the program as the integers NF1 to NF9, and are referred to within the program as NSYM1 to NSYM9.

The development of these codes is based directly on Table 4.1.9 and Section 4.3 of the International Tables.[16a] Table 4.1.9 was, however, specifically intended for X-ray diffraction studies of single crystals, and some modifications have been necessary in the derivation of the NSYM codes to make them meaningful in X-ray powder diffraction calculations. These modifications are noted below. Since the FLINT codes were compiled by Stocks[18] it has become necessary to update them.[16b]

The implications of the nine FLINT codes or NSYM codes are described fully in Appendix 4. There the NSYM codes are listed together with the conditions which the Miller indices h, k and ℓ must satisfy for the reflection to be allowed. The relevant portions of the short Hermann-Maugain space groups are also listed. The full space group symbols are not considered as these lead to 'redundant' conditions, i.e. conditions already catered for by the symmetry properties of the short symbol. Some features of these symbols are not strictly consistent between crystal classes, thus in the orthorhombic space group $Pca2_1$ (No. 29), 2_1 refers to a [001] screw axis, whereas in the tetragonal space group $I4_122$ (No. 98), 4_1 refers to a [001] screw axis.(6)

In broad outline, the operation of the NSYM codes is as follows:

NSYM1 covers the conditions imposed by the Bravais lattices, i.e. face and body centring, and various types of rhombohedral and hexagonal indexing. Conditions 8 and 10 do not apply directly to the space groups listed in the International Tables but they are included to present a complete picture; the program allows them to be input if required.

NSYM2 covers the restrictions imposed on reflections of the type Okℓ by the presence of {100} glide planes. Strictly it should apply not only to the orthorhombic systems but to the tetragonal and cubic systems. However, by convention, X-ray powder reflections for crystals of the cubic systems are described as hkO rather than Okℓ and so this type of reflection is considered under NSYM4. Similarly since FIREBIRD2 refers to hOℓ rather than its equivalent Okℓ in the tetragonal system, reflections of this type are considered under NSYM3 rather than under NSYM2.

NSYM3 considers the implications of (010) glide planes in a structure thus it considers reflections of the type hOℓ in the monoclinic (second setting), orthorhombic and tetragonal (see NSYM2) systems.

NSYM4 treats reflections of the type hkO and refers to the monoclinic (first setting), orthorhombic, tetragonal and cubic (see NSYM2) crystal systems. NSYM4 deals with the presence of (001) glide planes in a structure.

NSYM5 covers restrictions imposed on reflections of the type hhℓ and applies to the tetragonal, trigonal, hexagonal and cubic systems. NSYM5 covers the presence of {110} glide planes in a structure. Under NSYM5, code 2 covers not only the condition that ℓ must be even, but also the n glide condition which requires that (2h + ℓ) must be a multiple of four.

NSYM6 deals with reflections of the type hOO and treats the orthorhombic, tetragonal and cubic systems. It covers the effects of [100] screw axes in a structure.

NSYM7 covers the restrictions imposed on reflections of the type OkO by [010] screw axes in the monoclinic (second setting) and orthorhombic systems.

NSYM8 treats the implications of [001] screw axes on reflections of the type OOℓ in the monoclinic (first setting), orthorhombic and tetragonal systems and z screw axes in the hexagonal systems.

NSYM9 covers restrictions imposed on reflections of the type $h\bar{h}\ell$ (encountered in FIREBIRD2 as hOℓ) by $\{11\bar{2}0\}$ glide planes in the trigonal and hexagonal systems.

The values of NSYM corresponding to each space group are given in Appendix 5, and this table is accessed via the program NSYM from a disc file to the main program FIREBIRD3.

3.3 PROGRAM LISTING AND SUBROUTINE FUNCTIONS

The complete listing of the program FIREBIRD3 is given on micro-fiche (inside front cover). The role of the various constituent subroutines is summarised in Appendix 6. The actual instructions for compiling and running FIREBIRD3 on the UKAEA's Risley ICL 3980 computer are given in Appendix 7.

4. FORM OF INPUT

Data are input to the program from a standard 72 character record data file (in lieu of standard 80-column IBM cards). In general only one variable appears on a record (a single IBM card) except where stated below. With the exception of two variables, MAXNUM and NUMOBS, which are free format, all the variables are input in mixed format. In the input lists given below for FIREBIRD3 many variables are enclosed in square brackets. Whether or not such variables are input depends upon the program options specified. In the format specifications given below, F refers to a real number, I to an integer number, I0 to a free format integer and D0.0 to a floating point number. The lists which define the order of variables input, the names of the variables within the program, their respective formats, range of meaningful values assigned to each variable and their respective roles are given below.

Name of input variable	Format	Inclusive range of values	Role of variable
NO	I3	1 to 100	This record appears once only at the beginning of a set of examples. It defines the number of examples to be considered.
TITLE	-	6 records	These six records must appear for each example, although some or all of them may be blank. They contain up to 6 x 80 characters from the 256 character EBCDIC set which are necessary to define a 'title' for each example.
OUTPT1	I1	2	131 column wide output required corresponding to calculated and observed Bragg reflection positions.
		0	No output required which relates to Bragg reflection positions.
OUTPT2	I1	2	Output of interplanar angles, see the variable BALL which appears later, required. N.B. OUTPT2 set at 2 overrides all settings of OUTPT1.

Name of input variable	Format	Inclusive range of values	Role of variable
OUTPUT2 cont		1	Outputs blocks of Miller indices in a FIREFLY[1] compatible form.
		0	No OUTPT2 option specified
OBTHET	I2	3	The output data include the $\frac{1}{d}$, $\frac{1}{d_2}$, $\log_{10} d$, $\sin\theta$, $\frac{\sin\theta}{\lambda}$, the Nelson Riley[5] function, and $\cos^2\theta$; no observations are given.
		2	Observed Bragg angles given in $°2\theta$.
		1	Observed Bragg angles given in $°\theta$.
		0	No observed data given.
		-1	Observed Bragg angles given as d, interplanar spacings, in Å.
		-2	Observed Bragg angles given as $\sin^2\theta$ values.
NSYS	I3	15 to 2	Code defining the Laue symmetry group (see Appendix 2), NB NSYS overrides SG (see below) in program.
		1	Unallocated value.
		0	The program infers NSYS from SG and SETT (see later).
		-1	When NSYS is negative, NF1 to NF9 are read in (see below) but when NSYS is -1, LAUE SYMMETRY GROUP UNDEFINED is output. A 'dummy' value of SG must be input later, so that the necessary lattice parameters, 'A' etc. (see below) will be read in. In general SG would then be negative.
		-2 to -15	NF1 to NF9 are read (see above/below). These negative NSYS values are treated as their positive equivalents but no knowledge is required of the space group and SG may be read in later as 0 (when it is not referred to in the output).

Name of input variable	Format	Inclusive range of values	Role of variable
[NF1]		1 to 10	These codes (given on a single record) are only read when NSYS is negative. They define the conditions which limit the possible reflections from crystal system, see Appendix 2. Except when NSYS is negative these codes are referred to within the program which has access to NF1 to values of NF9 matched against each spacegroup (SG).
[NF2]		1 to 5	
[NF3]		1 to 5	
[NF4]		1 to 5	
[NF5]	9I2	1 to 3	
[NF6]		1 to 3	
[NF7]		1 to 2	
[NF8]		1 to 5	
[NF9]		1 to 2	
SG	I4	230 to 1	The space group applicable.
		0	No conditions are applied as to whether or not a reflection is allowed. If SG is 0, NSYS cannot be zero.
		-1 to -230	As for SG equals 1 to 230 but space group is not referred to in the output. NB. NSYS always overrides SG and SETT.
SETT	I1		Defines a crystal setting or axes thus:
		6	Refers the trigonal space groups 143 to 167 to hexagonal axes; it should be used for all hexagonal examples.
		3	Refers the trigonal space groups 143 to 167 to rhombohedral axes, where this is valid.
		2	Refers the monoclinic space groups 3 to 15 to their second setting (y-axis unique; BETA - see later - required in input) (the preferred I.U.Cr setting).
		1	Refers the monoclinic space groups 3 to 15 to their first setting (z-axis unique; GAMMA - see later - required later) (this setting is not recommended by the I.U.Cr).

Name of input variable	Format	Inclusive range of values	Role of variable
SETT Cont.		0	Space groups 3 to 15 are referred to their second setting (see above). Space groups 143 to 194 are referred to hexagonal axes (see above). For all other space groups SETT is read in, but ignored by the program.
REV	I1		Defines the setting used in the trigonal space group when hexagonal axes are used:
		0	Obverse setting applies.
		1	Reverse setting applies.
A [B] [C]	3F8.4	999.9999	The crystal lattice parameters a, b, c, α, β, γ are given on a single record; the particular ones input depend upon the cyrstal system e.g. the trigonal (rhombohedral setting) requires A and ALFA. The angles are given in degrees.
[ALFA] [BETA] [GAMMA]	3F9.4	180.0000 -180.0000	
NUMWAV	I2	13	The number of wavelengths used (the results are sorted in order of increasing Bragg angle).
WAVECO	I3	1 to 17	List of wavelength codes applied,(5) see Appendix 3.
		0	Unallocated value in program.
		-1 to -17	In the example given the program values of the X-ray wavelengths corresponding tc all the pcsitive WAVECO values are replaced by the following WAVECO values of WAV(N).
[WAVN(J)]	F11.8	99.99999999	List of wavelengths to be input (see WAVECO above).

Name of input variable	Format	Inclusive range of values	Role of variable
CUTOFF	F9.5		This value, which overrides MAXNO (see below) unless set at zero defines a limiting value beyond which no data are output, although the program actually manipulates values beyond this limit.
		1×10^{-5} to 180.00000	corresponding to OBTHET set at 2 (observations in °2θ input).
		1×10^{-5} to 90.00000	corresponding to OBTHET set at 1 or 0 (observations in °θ input or no observations input).
		999.99999 to 1×10^{-5}	corresponding to OBTHET set at -1 (observations input as d spacings).
		1×10^{-5} to 1.00000	corresponding to OBTHET set at -2 (observations input as $\sin^2\theta$ values).
MAXNO	I5	0 to 1000	The maximum number of Bragg reflections listed in order of ascending Bragg angle in the output. This value is not allowed to exceed 1000, although up to 10000 sets of Miller indices may be considered by the program. NB. MAXNO is over-ridden by CUTOFF so, for example, if MAXNO is 0 it is CUTOFF that decides the size of the output.
MAXNUM	I0	any positive integer	This value refers to the maximum number of increments allowed when the lattice parameters are varied incrementally (see main text). If MAXNUM is 0 it defaults to 20. NB. An incautious use of MAXNUM could prove very expensive!
NUMOBS	I0	0 and $\leq$ 1000	Data which compare observed and calculated information are only output when the number of matched data pairs within TOL (see below) is not less than NUMOBS.
TOL	F7.5	1.0	Observed and calculated data are considered to be matched when they differ by less than TOL in $\sin^2\theta$. (If OBTHET is 0 then TOL is, of course, 0).

Name of input variable	Format	Inclusive range of values	Role of variable
RHO	D0.0	0	Continue reading data at OBTH(J), see below.
		1	Uses Avogadro's number set within program at 6.022521×10^{23}.
		1.0	Resets Avogadro's number to the value assigned to RHO.
[TOAT]	I2	99	Number of types of atom within the unit cell.
[ATWT(I)] [NOAT(I)]	F9.5 F8.3	999.99999 9999.999	Atomic weight of Ith atomic species (on the same record as) the number of the Ith type of atom present within the unit cell (note this can be fractional to allow for different isotopic NB. I equals TOAT (see above).
OBTH(J) BWAV(J)	F9.5 I3	999.99999 17 to -17	List of matched pairs (on single records) of observed Bragg reflection positions (OBTHET above) and a wavelength code corresponding to WAVECO (see above). NB. This list must be in order or ascending θ. When BWAV(J) is set at zero, it and all subsequent observations are referred to the last wavelength code read in, and BWAV(J) need not be input again. OBTH(J) BWAV(J) set at zero terminates the reading of [OBTH(J)] [BWAV(J)] and data input recontinues at DELA.
[BALL]	I3	999	If OUTPT2 is set at 2, BALL is read here. It corresponds to the number of Miller indices following: however the program will only compute data which refer to a maximum of ten sets of reference MILLER INDICES.
[HR(IB)] [KR(IB)] [LR(IB)]	3I4	999	The number of records following is given by BALL (above). These records contain values of the Miller indices of the reference planes (see main text). The program reads all these records but only considers the first ten of them.

Name of input variable	Format	Inclusive range of values	Role of variable
DELA	F6.4		If DELA is 1.0000, the program moves on to the TITLE of the next example otherwise it also needs DELB etc., all on another record. DELA, DELB etc., correspond to the respective increments which will be applied to the variables A, B, C, ALFA, BETA and GAMMA, but note that values of DELA etc. are only input as are logically consistent with the values of NSYS, SG and SETT already input.
[DELB] [DELC] [DELALF] [DELBET] [DELGAM]	5F6.4 or as appro-priate	0.9999 to -0.9999	
[MAXA] [MAXB] [MAXC] [MAXALF] [MAXBET] [MAXGAM]	6F8.4 or as appro-priate	999.9999 to 001.0000 -180.0000 to 0180.0000	These data, all on one record, define the limits beyond which the operation of DELA, DELB, DELC, DELALF, DELBET and DELGAM cannot increase A, B, C, ALFA, BETA and GAMMA, as are logically consistent with the values of NSYS, SG and SETT already input.

4.1 RESTRICTIONS ON INPUT

Apart from the field widths described above the only restriction on the program is that the number of observations input cannot exceed 1000.

5. DESCRIPTIONS OF OUTPUT

The number of reflections output is limited to a maximum of 1000 irrespective of wavelength unless the number of reflections over the angular range considered is less than that value. The maximum angle considered is normally 90°θ but it can be restricted by the data input. Subject to the latter overriding conditions, a value can be inserted in the data input which limits the actual number of reflections in rhombohedral and triclinic examples before truncating the data for output.

Data may be output in several ways. Each reflection is always referred to in terms of its Miller indices, wavelength code number, θ, 2θ, $\sin^2\theta$, d and multiplicity. If required

(a) $\frac{1}{d}$, $\frac{1}{d^2}$, $\log_{10} d$, $\sin\theta$, $(\sin\theta)/\lambda$, the Nelson Riley function and

$\cos^2\theta$ may be output or

(b) it lists data which refer to actual observed reflection positions as follows: θ, 2θ, $\sin^2\theta$, d, as well as (calculated minus observed values) of θ, 2θ, $\sin^2\theta$ and d. Each observation is matched with the first calculated reflection which lies within a pre-assigned $\sin^2\theta$ window (TOL).

(c) it lists a reference plane and the interplanar angle between it and each calculated plane.

In addition blocks of h, k and ℓ can also be output in a form directly suitable for transcription as input to FIREFLY.[1]

Examples of the various forms of output, corresponding to various inputs, are given on micro-fiche as well as the FLINT codes.

6. CONCLUSIONS

The program has been tested thoroughly against a test set of examples, see the micro-fiche (inside front cover).

The program listing is given on micro-fiche (also inside front cover), and the role of the various subroutines is summarised in Appendix 6, Appendix 7 lists the instructions for compiling and running FIREBIRD3 on the Risley ICL 3980 computer. This program represents a final working version and no significant modifications are anticipated; although it is now realized that in the triclinic case the two equivalent reflections $hk\ell$ and $\bar{h}k\bar{\ell}$; $\bar{h}k\ell$ and $h\bar{k}\bar{\ell}$, etc are all output by FIREBIRD 3.

7. ACKNOWLEDGEMENTS

The authors are especially grateful to Mr C Stocks who initially derived the FLINT codes and wrote an ALGOL precursor to this program. They are also grateful to Mrs R Cooper who prepared the initial drafts of this program.

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8. APPENDIX 1
Crystallographic equations used

8.1 Volume of unit cell, V

$V = 2\,abc\,\sqrt{\{\sin s.\ \sin(s-\alpha).\ \sin(s-\beta).\ \sin(s-\gamma)\}}$

where $s = (\alpha + \beta + \gamma)/2$

8.2 Volume of reciprocal unit cell, V*

$V^* = a^*b^*c^*\ \sin\alpha^*\sin\beta^*\sin\gamma^*$

8.3 Reciprocal lattice parameters for the different crystal systems

(i) cubic (NSYS = 8 or 15)

$a^* = b^* = c^* = \frac{1}{a};\quad \alpha^* = \beta^* = \gamma^* = 90°$

(ii) rhombohedral (NSYS 7 or 14)

$a^* = b^* = c^* = (a^2 \sin\alpha)/V$, where $v = a^3\,[1-3\cos^2\alpha + 2\cos^3\alpha]^{\frac{1}{2}}$

$\cos\alpha^* = \cos\beta^* = \cos\gamma^* = -\cos\alpha/(1 + \cos\alpha)$

(iii) hexagonal (NSYS = 6, 11, 12 or 13)

$a^* = b^* = 2/a\sqrt{3};\ c^* = \frac{1}{c};\ \alpha^* = \beta^* = 90°;\ \gamma^* = 60°$

(iv) tetragonal (NSYS = 5 or 10)

$a^* = b^* = \frac{1}{a};\ c^* = \frac{1}{c};\ \alpha^* = \beta^* = \gamma^* = 90°$

(v) orthorhombic (NSYS = 4)

$a^* = \frac{1}{a};\ b^* = \frac{1}{b};\ c^* = \frac{1}{c};\ \alpha^* = \beta^* = \gamma^* = 90°$

(vi) monoclinic - 1st setting (NSYS = 9)

$a^* = 1/a \sin\gamma;\ b^* = 1/b \sin\gamma;\ c^* = \frac{1}{c};\ \alpha^* = \beta^* = 90°;\ \gamma^* = 180°-\gamma$

Note γ in the first setting = $(180 - \beta)$ where β is as in the 2nd setting; while a remains the same for both settings, but c in the 2nd setting becomes b in the 1st setting and vice versa.

monoclinic - 2nd setting (NSYS = 3)

$a^* = 1/a \sin\beta;\ b^* = \frac{1}{b};\ c^* = 1/c \sin\beta;\ \alpha^* = \gamma^* = 90°;\ \beta = 180°-\beta$

(vii) triclinic (NSYS = 2)

$a^* = bc.\sin\alpha/V;\ b^* = ca.\sin\beta/V;\ c^* = ab.\sin\gamma/V$

$$\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha;}{\sin\beta\sin\gamma} \qquad \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$$

$$\cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

8.4 Calculation of the Bragg angle, θ, via $\sin^2\theta$ for the:

(i) cubic system

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + \ell^2)$$

(ii) rhombohedral system

$$\sin^2\theta = \frac{\lambda^2[(h^2 + k^2 + \ell^2)\sin^2\alpha + 2(hk + k\ell + h\ell)(\cos^2\alpha - \cos\alpha)]}{4a^2(1 + 2\cos^3 - 3\cos^2\alpha)}$$

(iii) hexagonal system

$$\sin^2\theta = \frac{\lambda^2}{3a^2}(h^2 + hk + k^2) + \frac{\lambda^2}{4c^2}(\ell^2)$$

(iv) tetragonal system

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2) + \frac{\lambda^2}{4c^2}(\ell^2)$$

(v) orthorhombic system

$$\sin^2\theta = \frac{\lambda^2}{4a^2}h^2 + \frac{\lambda^2}{4b^2}k^2 + \frac{\lambda^2}{4c^2}\ell^2$$

(vi) monoclinic system (1st setting) - not preferred by the International Union of Crystallography

$$\sin^2\theta = \frac{\lambda^2}{4a^2\sin^2\gamma}h^2 - \frac{\lambda^2\cos\gamma}{2ab\sin^2\gamma}hk + \frac{\lambda^2}{4b^2\sin^2\gamma}k^2 + \frac{\lambda^2}{4c^2}\ell^2$$

monoclinic system (2nd setting) - preferred by the International Union of Crystallography

$$\sin^2\theta = \frac{\lambda^2}{4a^2\sin^2\beta}h^2 - \frac{\lambda^2\cos\beta}{2ac\sin^2\beta}h\ell + \frac{\lambda^2}{4c^2\sin^2\beta}\ell^2 + \frac{\lambda_2}{4b^2}k^2$$

(see 8.3 (vi) for the relationship between a, b, c, β and γ in these two settings

(vii) triclinic system

$$\sin^2\theta = \frac{\lambda^2}{4}[h^2a^{*2} + k^2b^{*2} + \ell^2c^{*2} + 2k\ell b^*c^*\cos\alpha^* + 2\ell hc^*a^*\cos\beta^* + \ell hka^*b^*\cos\gamma^*]$$

8.5 Interplanar angles for the triclinic system in the direct lattice between two planes with Miller Indices hkℓ and h'k'ℓ'

$$\cos\theta = hh'a^{*2} + kk'b^{*2} + \ell\ell'c^{*2} + (h\ell' + \ell k')\, b^*c^*\cos\alpha^* + (\ell h' + h\ell')\, c^*a^*\cos\beta^* + (hk' + h'k)\, a^*b^*\cos\gamma^* / \sqrt{(Q_{hk\ell}\, Q_{h'k'\ell'})}$$

where $Q_{hk\ell}$ is given by

$$Q_{hk\ell} = h^2a^{*2} + k^2b^{*2} + \ell^2c^{*2} + 2k\ell b^*c^*\cos\alpha^* + 2\ell hc^*a^*\cos\beta^* + 2kha^*b^*\cos\gamma^*$$

9. APPENDIX 2

The relationship between the NSYS codes and the crystal symmetry

Space groups	Crystal setting or axes	Point groups	Laue-symmetry group	Crystal system	NSYS code in FIREFLY
1-2		1, $\bar{1}$	$\bar{1}$	triclinic	2
3-15	1st setting (z-axis unique; GAMMA input)	2, m, 2/m	2/m	monoclinic	9
3-15	2nd setting or unspecified (y-axis unique; BETA input)	2, m, 2/m	2/m	monoclinic	3
16-74		222, mm2, mmm	mmm	orthorhombic	4
75-88		4, $\bar{4}$, 4/m	4/m	tetragonal	5
89-142		422, 4mm, $\bar{4}$2m , 4/mmm	4/mmm	tetragonal	10
143-148	rhombohedral or unspecified	3, $\bar{3}$	$\bar{3}$	trigonal	7
143-148	hexagonal	3, $\bar{3}$	$\bar{3}$	trigonal	6
149-167	rhombohedral or unspecified	32, 3m, $\bar{3}$m	$\bar{3}$m	trigonal	14
149-167	hexagonal	32, 3m, $\bar{3}$m	$\bar{3}$m	trigonal	11
168-176		6, $\bar{6}$, 6/m	6/m	hexagonal	12
177-194		622, 6mm, $\bar{6}$m2, 6/mmm	6/mmm	hexagonal	13
195-206		23, m3	m3	cubic	8
207-230		432, $\bar{4}$3m, m3m	m3m	cubic	15

10. APPENDIX 3

List of X-ray wavelengths pre-set within FIREBIRD3 and the corresponding input/output data codes

X-radiation	Corresponding WAVECO code	Wavelength applied (Å)
Cu $K\alpha_1$	1	1.54050
Cu $K\alpha_2$	2	1.54434
Cu $K\alpha$ (weighted mean)	3	1.54178
Cu $K\beta$	4	1.39217
Cr $K\alpha_1$	5	2.28962
Cr $K\alpha_2$	6	2.29352
Cr $K\alpha$ (weighted mean)	7	2.29092
Fe $K\alpha_1$	8	1.93597
Fe $K\alpha_2$	9	1.93991
Fe $K\alpha$ (weighted mean)	10	1.93728
Co $K\alpha_1$	11	1.78890
Co $K\alpha_2$	12	1.79279
Co $K\alpha$ (weighted mean)	13	1.79020
Mo $K\alpha_1$	14	0.70926
Mo $K\alpha_2$	15	0.71354
Ag $K\alpha_1$	16	0.55941
Ag $K\alpha_2$	17	0.56381

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11. APPENDIX 4

A full description of the operation of the NSYM codes

NSYM 1 (which defines the Bravais lattice) is first considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	None	P (primitive) or R (rhombohedral indexed with rhombohedral axes) or C (hexagonal, as in 1935 edition of International Tables for Crystal Structure Determination, Volume I)
2	$h + k + \ell = 2n$	I (body centred)
3	$h + k = 2n$	C (c face-centred)
4	$h + \ell = 2n$	B (b face-centred)
5	$k + \ell = 2n$	A (a face-centred)
6	$h + k = 2n$	
	$k + \ell = 2n$	F (all face centred)
	$h + \ell = 2n$	
7	$-h + k + \ell = 3n$	R (rhombohedral, indexed on hexagonal axes - obverse position)
8	$h + k + \ell = 3n$	P or C [see above] (hexagonal indexed on rhombohedral axes)
9	$h - k + \ell = 3n$	R (rhombohedral, indexed on hexagonal axes - reverse position)
10	$h - k = 3n$	H (hexagonal, triple cell)

Then if the crystal system is orthorhombic for Okℓ (including Okk) NSYM2 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No {100} glide planes present
2	k = 2n	(P) or (A) or (I) then b-- or -b-
3	ℓ = 2n	(P) or (C) then c-- or -c-
4	k + ℓ = 2n	(P) then n-- or -n-
5	k + ℓ = 4n	(F) then d-- or d-

Then if the crystal system is monoclinic (second setting), orthorhombic, or tetragonal or cubic for h0ℓ (which includes h0h) NSYM 3 is considered.

Code	Conditions operating h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No (010) glide planes present
2	h = 2n	(P) or (A) or (I) then -a- (P) then (-)-b-
3	ℓ = 2n	(P) or (C) or (I) then (-)-b- or(-)-c- or (p)c-
4	h + ℓ = 2n	(P) then (-)-n-
5	h + ℓ = 4n	(F) then -d-

Then if the crystal system is monoclinic (first setting), orthorhombic, or tetragonal or cubic for hk0 (including hh0), NSYM 4 is considered.

Code	Conditions operating h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No (001) glide planes present
2	h = 2n	(P) or (C) or (I) --a; or (P--a; or I (-)a--; or (P) or (I)a
3	k = 2n	(P) b- or (P) -b
4	h + k = 2n	(P)--n; or P(-) -n-; or (P) n; or (P)-n--
5	h + k = 4n	(F)--d; or (F)d

Then if the crystal is tetragonal, trigonal, hexagonal or cubic for hhℓ (which includes hh0 and hhh, but not 00h), NSYM 5 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No $\{1\bar{1}0\}$ glide planes present
2	ℓ = 2n	(P)--c; or (P)(-)--c; or (P)--n; or (R) -c
3	2h + ℓ = 4n	(I)--d; or (I)(-)--d
4	h = 2n and ℓ = 2n	
5	ℓ = 3n	

Then if the system is orthorhombic, tetragonal or cubic for h00, NSYM 6 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No 100 screw axes present
2	h = 2n	(P) 2_1-- or (I)-2_1; or (P)4_2
3	h = 4n	(R) or (F) or (I) 4_1--; or (P)4_3--

Then if the system is monoclinic (second setting) or orthorhombic for 0k0, NSYM 7 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No [010] screw axes present
2	k = 2n	(I)2_1--; or (P)-2_1-

Then if the system is monoclinic (first setting), orthorhombic, tetragonal, trigonal or hexagonal for 00ℓ, NSYM 8 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	Neither [001] nor z screw axes present
2	ℓ = 2n	(P)2_1 or 2_1- or 4_2 or 4_2- or (P)--2_1 (P)6_3 or 6_3- or 6_3--
3	ℓ = 3n	(P)3_1 or 3_1-b-- or 3_2 or 3_2- or (P)6_2 or 6_2-- or 6_4 or 6_4--
4	ℓ = 4n	(P) or (I)4_1; or (P)4_3; or (I)4_1; or (P or I)4_1--; or (P)4_3--
5	ℓ = 6n	(P)6_1 or 6_5; or (P)6_1-- or 6_5--

Finally if the system is trigonal or hexagonal for $h\bar{h}\ell$ (which corresponds to h0ℓ) NSYM 9 is considered.

Code	Conditions operating on h, k and ℓ	Relevant portion of short space group symbol and comments
1	No conditions	No $\{11\bar{2}0\}$ glide planes present
2	ℓ = 2n	(R)-c or (P)-c- or (P)(-)-c-

12. APPENDIX 5

A description of the NSYM and NSYS codes for each of the 230 space groups

Space group number	Short space group symbol	NSYM codes									Short point group symbol	NSYS code
		NF1	NF2	NF3	NF4	NF5	NF6	NF7	NF8	NF9		
TRICLINIC												
1	P1	1	1	1	1	1	1	1	1	1	1	2
2	$P\bar{1}$	1	1	1	1	1	1	1	1	T	$\bar{1}$	2
MONOCLINIC												
3 (1st setting)	P2	1	1	1	1	1	1	1	1	1	2	9
3 (2nd ")	P2	1	1	1	1	1	1	1	1	1	2	3
4 (1st ")	$P2_1$	1	1	1	1	1	1	1	2	1	2	9
4 (2nd ")	$P2_1$	1	1	1	1	1	1	2	1	1	2	3
5 (1st ")	B2	4	1	1	1	1	1	1	1	1	2	9
5 (2nd ")	C2	3	1	1	1	1	1	1	1	1	2	3
6 (1st ")	Pm	1	1	1	1	1	1	1	1	1	m	9
6 (2nd ")	Pm	1	1	1	1	1	1	1	1	1	m	3
7 (1st ")	Pb	1	1	1	3	1	1	1	1	1	m	9
7 (2nd ")	Pc	1	1	3	1	1	1	1	1	1	m	3
8 (1st ")	Bm	4	1	1	1	1	1	1	1	1	m	9
8 (2nd ")	Cm	3	1	1	1	1	1	1	1	1	m	3
9 (1st ")	Bb	4	1	1	3	1	1	1	1	1	m	9
9 (2nd ")	Cc	3	1	3	1	1	1	1	1	1	m	3
10 (1st ")	P2/m	1	1	1	1	1	1	1	1	1	2/m	9
10 (2nd ")	P2/m	1	1	1	1	1	1	1	1	1	2/m	3
11 (1st ")	$P2_1/m$	1	1	1	1	1	1	1	2	1	2/m	9
11 (2nd ")	$P2_1/m$	1	1	1	1	1	1	2	1	1	2/m	3
12 (1st ")	B2/m	4	1	1	1	1	1	1	1	1	2/m	9
12 (2nd ")	C2/m	3	1	1	1	1	1	1	1	1	2/m	3
13 (1st ")	P2/b	1	1	1	3	1	1	1	1	1	2/m	9
13 (2nd ")	P2/c	1	1	3	1	1	1	1	1	1	2/m	3
14 (1st ")	$P2_1/b$	1	1	1	3	1	1	1	2	1	2/m	9
14 (2nd ")	$P2_1/c$	1	1	3	1	1	1	2	1	1	2/m	3
15 (1st ")	B2/b	4	1	1	3	1	1	1	1	1	2/m	9
15 (2nd ")	C2/c	3	1	3	1	1	1	1	1	1	2/m	3
ORTHORHOMBIC												
16	P222	1	1	1	1	1	1	1	1	1	222	4
17	$P222_1$	1	1	1	1	1	1	1	2	1	222	4
18	$P2_12_12$	1	1	1	1	1	2	2	1	1	222	4
19	$P2_12_12_1$	1	1	1	1	1	2	2	2	1	222	4
20	$C222_1$	3	1	1	1	1	1	1	2	1	222	4
21	C222	3	1	1	1	1	1	1	1	1	222	4
22	F222	6	1	1	1	1	1	1	1	1	222	4
23	I222	2	1	1	1	1	1	1	1	1	222	4
24	$I2_12_12_1$	2	1	1	1	1	1	1	1	1	222	4
25	Pmm2	1	1	1	1	1	1	1	1	1	mm2	4
26	$Pmc2_1$	1	1	3	1	1	1	1	1	1	mm2	4
27	Pcc2	1	3	3	1	1	1	1	1	1	mm2	4
28	Pma2	1	1	2	1	1	1	1	1	1	mm2	4
29	$Pca2_1$	1	3	2	1	1	1	1	1	1	mm2	4
30	Pnc2	1	4	3	1	1	1	1	1	1	mm2	4
31	$Pmn2_1$	1	1	4	1	1	1	1	1	1	mm2	4
32	Pba2	1	2	2	1	1	1	1	1	1	mm2	4
33	$Pna2_1$	1	4	2	1	1	1	1	2	1	mm2	4
34	Pnn2	1	4	4	1	1	1	1	1	1	mm2	4
35	Cmm2	3	1	1	1	1	1	1	1	1	mm2	4
36	$Cmc2_1$	3	1	3	1	1	1	1	1	1	mm2	4
37	Ccc2	3	3	3	1	1	1	1	1	1	mm2	4
38	Amm2	5	1	1	1	1	1	1	1	1	mm2	4
39	Abm2	5	2	1	1	1	1	1	1	1	mm2	4
40	Ama2	5	1	2	1	1	1	1	1	1	mm2	4
41	Aba2	5	2	2	1	1	1	1	1	1	mm2	4
42	Fmm2	6	1	1	1	1	1	1	1	1	mm2	4
43	Fdd2	6	5	5	1	1	1	1	1	1	mm2	4
44	Imm2	2	1	1	1	1	1	1	1	1	mm2	4
45	Iba2	2	2	2	1	1	1	1	1	1	mm2	4

Continued ...

Appendix 5 continued

Space group number	Short space group symbol	NSYM codes									Short point group symbol	NSYS code
		NF1	NF2	NF3	NF4	NF5	NF6	NF7	NF8	NF9		
ORTHORHOMBIC (continued)												
46	Ima2	2	1	2	1	1	1	1	1	1	mm2	4
47	Pmmm	1	1	1	1	1	1	1	1	1	mmm	4
48	Pnnn	1	4	4	4	1	1	1	1	1	mmm	4
49	Pccm	1	3	3	1	1	1	1	1	1	mmm	4
50	Pban	1	2	2	4	1	1	1	1	1	mmm	4
51	Pmma	1	1	1	2	1	1	1	1	1	mmm	4
52	Pnna	1	4	4	2	1	1	1	1	1	mmm	4
53	Pmna	1	1	4	2	1	1	1	1	1	mmm	4
54	Pcca	1	3	3	2	1	1	1	1	1	mmm	4
55	Pbam	1	2	2	1	1	1	1	1	1	mmm	4
56	Pccn	1	3	3	4	1	1	1	1	1	mmm	4
57	Pbcm	1	2	3	1	1	1	1	1	1	mmm	4
58	Pnnm	1	4	4	1	1	1	1	1	1	mmm	4
59	Pmmn	1	1	1	4	1	1	1	1	1	mmm	4
60	Pbcn	1	2	3	4	1	1	1	1	1	mmm	4
61	Pbca	1	2	3	2	1	1	1	1	1	mmm	4
62	Pnma	1	4	1	2	1	1	1	1	1	mmm	4
63	Cmcm	3	1	3	1	1	1	1	1	1	mmm	4
64	Cmca	3	1	3	2	1	1	1	1	1	mmm	4
65	Cmmm	3	1	1	1	1	1	1	1	1	mmm	4
66	Cccm	3	3	3	1	1	1	1	1	1	mmm	4
67	Cmma	3	1	1	2	1	1	1	1	1	mmm	4
68	Ccca	3	3	3	2	1	1	1	1	1	mmm	4
69	Fmmm	6	1	1	1	1	1	1	1	1	mmm	4
70	Fddd	6	5	5	5	1	1	1	1	1	mmm	4
71	Immm	2	1	1	1	1	1	1	1	1	mmm	4
72	Ibam	2	2	2	1	1	1	1	1	1	mmm	4
73	Ibca	2	2	3	2	1	1	1	1	1	mmm	4
74	Imma	2	1	1	2	1	1	1	1	1	mmm	4
TETRAGONAL												
75	P4	1	1	1	1	1	1	1	1	1	4	5
76	$P4_1$	1	1	1	1	1	1	1	4	1	4	5
77	$P4_2$	1	1	1	1	1	1	1	2	1	4	5
78	$P4_3$	1	1	1	1	1	1	1	4	1	4	5
79	I4	2	1	1	1	1	1	1	1	1	4	5
80	$I4_1$	2	1	1	1	1	1	1	4	1	$\bar{4}$	5
81	$P\bar{4}$	1	1	1	1	1	1	1	1	1	$\bar{4}$	5
82	$I\bar{4}$	2	1	1	1	1	1	1	1	1	$\bar{4}$	5
83	P4/m	1	1	1	1	1	1	1	1	1	4/m	5
84	$P4_2/m$	1	1	1	1	1	1	1	2	1	4/m	5
85	P4/n	1	1	1	4	1	1	1	1	1	4/m	5
86	$P4_2/n$	1	1	1	4	1	1	1	2	1	4/m	5
87	I4/m	2	1	1	1	1	1	1	1	1	4/m	5
88	$I4_1/a$	2	1	1	2	1	1	1	4	1	4/m	5
89	P422	1	1	1	1	1	1	1	1	1	422	10
90	$P42_12$	1	1	1	1	1	2	1	1	1	422	10
91	$P4_122$	1	1	1	1	1	1	1	4	1	422	10
92	$P4_12_12$	1	1	1	1	1	2	1	4	1	422	10
93	$P4_222$	1	1	1	1	1	1	1	2	1	422	10
94	$P4_22_12$	1	1	1	1	1	2	1	2	1	422	10
95	$P4_322$	1	1	1	1	1	1	1	4	1	422	10
96	$P4_32_12$	1	1	1	1	1	2	1	4	1	422	10
97	I422	2	1	1	1	1	1	1	1	1	422	10
98	$I4_122$	2	1	1	1	1	1	1	4	1	422	10
99	P4mm	1	1	1	1	1	1	1	1	1	4mm	10
100	P4bm	1	1	2	1	1	1	1	1	1	4mm	10
101	$P4_2cm$	1	1	3	1	1	1	1	1	1	4mm	10
102	$P4_2nm$	1	1	4	1	1	1	1	1	1	4mm	10
103	P4cc	1	1	3	1	2	1	1	1	1	4mm	10
104	P4nc	1	1	4	1	2	1	1	1	1	4mm	10

Continued ...

Appendix 5 continued

Space group number	Short space group symbol	NSYM codes									Short point group symbol	NSYS code
		NF1	NF2	NF3	NF4	NF5	NF6	NF7	NF8	NF9		
TETRAGONAL (Continued)												
105	$P4_2mc$	1	1	1	1	2	1	1	1	1	4mm	10
106	$P4_2bc$	1	1	2	1	2	1	1	1	1	4mm	10
107	I4mm	2	1	1	1	1	1	1	1	1	4mm	10
108	I4cm	2	1	3	1	1	1	1	1	1	4mm	10
109	$I4_1md$	2	1	1	1	3	1	1	1	1	4mm	10
110	$I4_1cd$	2	1	3	1	3	1	1	1	1	$\bar{4}$mm	10
111	$P\bar{4}2_1m$	1	1	1	1	1	1	1	1	1	$\bar{4}$2m	10
112	$P\bar{4}2c$	1	1	1	1	2	1	1	1	1	$\bar{4}$2m	10
113	$P\bar{4}2_1m$	1	1	1	1	1	2	1	1	1	$\bar{4}$2m	10
114	$P\bar{4}2_1c$	1	1	1	1	2	2	1	1	1	$\bar{4}$2m	10
115	$P\bar{4}m2$	1	1	1	1	1	1	1	1	1	$\bar{4}$2m	10
116	$P\bar{4}c2$	1	1	3	1	1	1	1	1	1	$\bar{4}$2m	10
117	$P\bar{4}b2$	1	1	2	1	1	1	1	1	1	$\bar{4}$2m	10
118	$P\bar{4}n2$	1	1	4	1	1	1	1	1	1	$\bar{4}$2m	10
119	$I\bar{4}m2$	2	1	1	1	1	1	1	1	1	$\bar{4}$2m	10
120	$I\bar{4}c2$	2	1	3	1	1	1	1	1	1	$\bar{4}$2m	10
121	$I\bar{4}2m$	2	1	1	1	1	1	1	1	1	$\bar{4}$2m	10
122	$I\bar{4}2d$	2	1	1	1	3	1	1	1	1	$\bar{4}$2m	10
123	P/4mmm	1	1	1	1	1	1	1	1	1	4/mmm	10
124	P4/mcc	1	1	3	1	2	1	1	1	1	4/mmm	10
125	P4/nbm	1	2	1	4	1	1	1	1	1	4/mmm	10
126	P4/nnc	1	4	1	4	2	1	1	1	1	4/mmm	10
127	P4/mbm	1	2	1	1	1	2	1	1	1	4/mmm	10
128	P4/mnc	1	4	1	1	2	2	1	1	1	4/mmm	10
129	P4/nmm	1	1	1	4	1	2	1	1	1	4/mmm	10
130	P4/ncc	1	3	1	4	2	2	1	2	1	4/mmm	10
131	$P4_2/mmc$	1	1	1	1	2	1	1	2	1	4/mmm	10
132	$P4_2/mcm$	1	3	1	1	1	1	1	2	1	4/mmm	10
133	$P4_2/nbc$	1	2	1	4	2	2	1	2	1	4/mmm	10
134	$P4_2/nnm$	1	4	1	4	1	2	1	2	1	4/mmm	10
135	$P4_2/mbc$	1	2	1	1	2	2	1	2	1	4/mmm	10
136	$P4_2/mnm$	1	4	1	1	1	2	1	2	1	4/mmm	10
137	$P4_2/nmc$	1	1	1	4	2	2	1	2	1	4/mmm	10
138	$P4_2/ncm$	1	3	1	4	1	2	1	2	1	4/mmm	10
139	$I4/mmm$	2	1	1	1	1	2	1	2	1	4/mmm	10
140	I4/mcm	2	3	1	1	1	2	1	2	1	4/mmm	10
141**	$I4_1/amd$	2	3	1	2	3	2	1	4	1	4/mmm	10
142**	$I4_1/acd$	2	3	1	2	3	2	1	4	1	4/mmm	10
TRIGONAL												
143	P3	1	1	1	1	1	1	1	1	1	3	6
144	$P3_1$	1	1	1	1	1	1	1	3	1	3	6
145	$P3_2$	1	1	1	1	1	1	1	3	1	3	6
146 (rhombohedral axes)	R3	1	1	1	1	1	1	1	1	1	3	7
146 (hexagonal axes)	R3	7	1	1	1	5	1	1	1	1	3	6
147	$P\bar{3}$	1	1	1	1	1	1	1	1	1	$\bar{3}$	6
148 (rhombohedral axes)	$R\bar{3}$	1	1	1	1	1	1	1	1	1	$\bar{3}$	7
148 (hexagonal axes)	$R\bar{3}$	7	1	1	1	5	1	1	1	1	$\bar{3}$	6
149	P312	1	1	1	1	1	1	1	1	1	312	11
150	P321	1	1	1	1	1	1	1	1	1	321	11
151	$P3_112$	1	1	1	1	1	1	1	3	1	312	11
152	$P3_121$	1	1	1	1	1	1	1	3	1	321	11
153	$P3_212$	1	1	1	1	1	1	1	3	1	312	11
154	$P3_221$	1	1	1	1	1	1	1	3	1	321	11
155 (rhombohedral axes)	$R3\bar{2}$	1	1	1	1	1	1	1	1	1	32	14
155 (hexagonal axes)	R32	7	1	1	1	5	1	1	1	1	32	11
156	$P3m_1$	1	1	1	1	1	1	1	1	1	3m1	11
157	P31m	1	1	1	1	1	1	1	1	1	31m	11
158	P3c1	1	1	1	1	1	1	1	2	2	3m1	11
159	P31c	1	1	1	1	2	1	1	2	1	31m	11

Continued ...

Appendix 5 continued

Space group number	Short space group symbol	NSYM codes									Short point group symbol	NSYS code
		NF1	NF2	NF3	NF4	NF5	NF6	NF7	NF8	NF9		
TRIGONAL (continued)												
160 (rhombohedral axes)	R3m	1	1	1	1	1	1	1	1	1	3m	14
160 (hexagonal axes)	R3m	7	1	1	1	5	1	1	1	1	3m	11
161 (rhombohedral axes)	R3c	1	1	1	1	4	1	1	1	1	3m	14
161 (hexagonal axes)	R3c	7	1	1	1	5	1	1	5	2	3m	11
162	P$\bar{3}$1m	1	1	1	1	1	1	1	1	1	$\bar{3}$1m	11
163	P$\bar{3}$1c	1	1	1	1	2	1	1	2	1	$\bar{3}$1m	11
164	P$\bar{3}$m1	1	1	1	1	1	1	1	1	1	$\bar{3}$m1	11
165	P$\bar{3}$c1	1	1	1	1	1	1	1	2	2	$\bar{3}$m1	11
166 (rhombohedral axes)	R$\bar{3}$m	1	1	1	1	1	1	1	1	1	$\bar{3}$m	14
166 (hexagonal axes)	R$\bar{3}$m	7	1	1	1	5	1	1	1	1	$\bar{3}$m	11
167 (rhombohedral axes)	R$\bar{3}$c	1	1	1	1	2	1	1	1	1	$\bar{3}$m	14
167 (hexagonal axes)	R$\bar{3}$c	7	1	1	1	5	1	1	5	2	$\bar{3}$m	11
HEXAGONAL												
168	P6	1	1	1	1	1	1	1	1	1	6	12
169	P6_1	1	1	1	1	1	1	1	5	1	6	12
170	P6_5	1	1	1	1	1	1	1	5	1	6	12
171	P6_2	1	1	1	1	1	1	1	3	1	6	12
172	P6_4	1	1	1	1	1	1	1	3	1	6	12
173	P6_3	1	1	1	1	1	1	1	2	1	6	12
174	P$\bar{6}$	1	1	1	1	1	1	1	1	1	$\bar{6}$	12
175	P6/m	1	1	1	1	1	1	1	1	1	6/m	12
176	P6_3/m	1	1	1	1	1	1	1	2	1	6/m	12
177	P622	1	1	1	1	1	1	1	1	1	622	13
178	P$6_1$22	1	1	1	1	1	1	1	5	1	622	13
179	P$6_5$22	1	1	1	1	1	1	1	5	1	622	13
180	P$6_2$22	1	1	1	1	1	1	1	3	1	622	13
181	P$6_4$22	1	1	1	1	1	1	1	3	1	622	13
182	P$6_3$22	1	1	1	1	1	1	1	2	1	622	13
183	P6mm	1	1	1	1	1	1	1	1	1	6mm	13
184	P6cc	1	1	1	1	2	1	1	2	2	6mm	13
185	P6_3cm	1	1	1	1	1	1	1	2	2	6mm	13
186	P6_3mc	1	1	1	1	2	1	1	2	1	6mm	13
187	P$\bar{6}$m2	1	1	1	1	1	1	1	1	1	$\bar{6}$m2	13
188	P$\bar{6}$c2	1	1	1	1	1	1	1	2	2	$\bar{6}$m2	13
189	P$\bar{6}$2m	1	1	1	1	1	1	1	1	1	$\bar{6}$2m	13
190	P$\bar{6}$2c	1	1	1	1	2	1	1	2	1	$\bar{6}$2m	13
191	P6/mmm	1	1	1	1	1	1	1	1	1	6/mmm	13
192	P6/mcc	1	1	1	1	2	1	1	2	2	6/mmm	13
193	P6_3/mcm	1	1	1	1	1	1	1	2	2	6/mmm	13
194	P6_3/mmc	1	1	1	1	2	1	1	2	1	6/mmm	13
CUBIC												
195	P23	1	1	1	1	1	1	1	1	1	23	8
196	F23	6	1	1	1	1	1	1	1	1	23	8
197	I23	2	1	1	1	1	1	1	1	1	23	8
198	P2_13	1	1	1	1	1	2	1	1	1	23	8
199	I2_13	2	1	1	1	1	1	1	1	1	23	8
200	Pm$\bar{3}$	1	1	1	1	1	1	1	1	1	m$\bar{3}$	8
201	Pn$\bar{3}$	1	1	1	4	1	2	1	1	1	m$\bar{3}$	8
202	Fm$\bar{3}$	6	1	1	1	1	1	1	1	1	m$\bar{3}$	8
203	Fd$\bar{3}$	6	1	1	5	1	3	1	1	1	m$\bar{3}$	8
204	Im3	2	1	1	1	1	1	1	1	1	m3	8

Appendix 5 continued

Space group number	Short space group symbol	NSYM codes									Short point group symbol	NSYS code
		NF1	NF2	NF3	NF4	NF5	NF6	NF7	NF8	NF9		
CUBIC (continued)												
205	Pa3	1	1	1	2	1	2	1	1	1	m3	8
206	Ia3	2	1	1	2	1	1	1	1	1	m3	8
207	P432	1	1	1	1	1	1	1	1	1	432	15
208	$P4_232$	1	1	1	1	1	2	1	1	1	432	15
209	F432	6	1	1	1	1	1	1	1	1	432	15
210	$F4_132$	6	1	1	1	1	3	1	1	1	432	15
211	I432	2	1	1	1	1	1	1	1	1	432	15
212	$P4_332$	1	1	1	1	1	3	1	1	1	432	15
213	$P4_132$	1	1	1	1	1	3	1	1	1	432	15
214	$I4_132$	2	1	1	1	1	3	1	1	1	432	15
215	$P\bar{4}3m$	1	1	1	1	1	1	1	1	1	$\bar{4}3m$	15
216	$F\bar{4}3m$	6	1	1	1	1	1	1	1	1	$\bar{4}3m$	15
217	$I\bar{4}3m$	2	1	1	1	1	1	1	1	1	$\bar{4}3m$	15
218	$P\bar{4}3n$	1	1	1	1	2	2	1	1	1	$\bar{4}3m$	15
219	$F\bar{4}3c$	6	1	1	1	2	1	1	1	1	$\bar{4}3m$	15
220	$I\bar{4}3d$	2	1	1	1	3	3	1	1	1	$\bar{4}3m$	15
221	$Pm\bar{3}m$	1	1	1	1	1	1	1	1	1	$m\bar{3}m$	15
222	$Pn\bar{3}$	1	1	1	4	2	2	1	1	1	$m\bar{3}m$	15
223	$Pm\bar{3}n$	1	1	1	1	2	2	1	1	1	$m\bar{3}m$	15
224	$Pn\bar{3}m$	1	1	1	1	1	2	1	1	1	$m\bar{3}m$	15
225	$Fm\bar{3}m$	6	1	1	1	1	1	1	1	1	$m\bar{3}m$	15
226	$Fm\bar{3}c$	6	1	1	1	2	1	1	1	1	$m\bar{3}m$	15
227	$Fd\bar{3}m$	6	1	1	5	1	3	1	1	1	$m\bar{3}m$	15
228	$Fd\bar{3}c$	6	1	1	5	2	3	1	1	1	$m\bar{3}m$	15
229	$Im\bar{3}m$	2	1	1	1	1	1	1	1	1	$m\bar{3}m$	15
230	$Ia\bar{3}d$	2	1	1	2	3	3	1	1	1	$m\bar{3}m$	15

13. APPENDIX 6

Role of the various subroutines used in FIREBIRD3

File No.	Operation
S/R FB1	Main control and starting routine.
S/R FB2	To read in data off the parameter cards.
S/R FB3	To calculate the values of the a* b* c* α* etc.
S/R FB4	To output and calculate the parameters and dimensions of the cell.
S/R FB5	To write the headings for the output of the Bragg angles.
S/R FB6	To work out the Bragg angles and to eliminate unnecessary reflections for the cube.
S/R FB7	To work out the Bragg angles and to eliminate unnecessary reflections for the triclinic case.
S/R FB8	To work out the Bragg angles and to eliminate unnecessary reflections for the trigonal/rhombohedral case.
S/R FB9	To work out the Bragg angles and to eliminate unnecessary reflections for the trigonal/hexagonal case.
S/R FB10	To work out the Bragg angles and to eliminate unnecessary reflections for the monoclinic case.
S/R FB11	To work out the Bragg angles and to eliminate unnecessary reflections for the orthorhombic case.
S/R FB12	To work out the Bragg angles for the hexagonal crystal system. Relevant HKL combinations are created and their validity is then checked, if required, by S/R FB19.
S/R FB13	To work out the Bragg angles and to eliminate unnecessary reflections for the tetragonal case.
S/R FB14	To sort out the Bragg angles into ascending order.
S/R FB15	To output the calculated and observed Bragg angles.
S/R FB16	To output a table of hkl's for input to the program "FIREFLY".
S/R FB17	To compare the reference plane Miller indices and to calculate the interplanar angle.
S/R FB18	To modify and produce combinations of unit cell parameter values for each crystal system. Parameters that may be modified depend on the crystal system, but are modified independently of each other by user supplied increments until the limiting value (user supplied) is reached.

S/R FB19 To eliminate unwanted hkl's using given conditions, defined by the NSYM codes.

S/R FB20 To identify the wavelengths using the given wave code.

S/R FB21 To determine the dimensions of the crystal, which have not been supplied.

S/R FB22 To determine the value of NSYS for given values of SG and SETT.

S/R FB23 Function used in the S/R FB24.

S/R FB24 Infers the multiplicity of a reflection on the basis of the Laue group and its Miller indices.

S/R FB25 To create hkl values of ascending order, k may not be > h, and l may not be > k.

S/R FB26 To calculate the limiting h value for a crystal system.

S/R FB27 Retrieves results which have been output to disc by S/R FB15.

14. APPENDIX 7

Instructions for compiling and running FIREBIRD 3 on the UKAEA's Risley ICL 3980 Computer

1. The Program Modules

FIREBIRD comprises a main program, 26 subroutines and 1 function. For convenience these routines are stored in 7 files in the library :RFLBOF.FIREBIRDSCE. These are:

FIRE1, FIRE2, FIRE3, FIRE4, FIRE5, FIRE6 and FIRE7

The main program and subroutines FB2 and FB3 are stored in FIRE1.
Subroutines FB4, FB5 and FB6 are stored in FIRE2.
Subroutines FB7, FB8 and FB9 are stored in FIRE3.
Subroutines FB10, FB11, FB12 and FB13 are stored in FIRE4.
Subroutines FB14, FB15, FB16 and FB17 are stored in FIRE5.
Subroutines FB18, FB19 and FB20 are stored in FIRE6.
Subroutines FB21, FB22, FB23, FB24, FB25, FB26 and FB27 and the function ASIN are stored in FIRE7.

2. Compiling the program

If any of the program subroutines are modified, then the file(s) containing the modified subroutines will have to be compiled. For example, suppose FB5 and FB15 are modified, then the following commands, typed in during a MAC session of user :RFLBOF, will compile the program.

```
PRO(FIREBIRD)
COPT(NONE,MESSAGES=NOCOMMENTS)
FTN(C,FIRE2)
FTN(C,FIRE5)
COLLECT(COLLSCL)
```

Any compiler comments at the end of the compilation can be ignored. For details on the ICL 3980 commands used, refer to the 3980 Users' Manual.

3. Running the program

The following file is needed to run FIREBIRD on the ICL 3980.

```
****
JOB(:RFLBOF.jobname,ACC=account number)
DATA
WOR(9,L,100,500)
ASS(:RFLBOF.FLINTDATA,28)
OUT(MAX=3000)
ROPT(TRIES=100,CONT=YES)
USING(COLLOMF)
ENTER FIREBIRD
data
ENDJOB
****
```

If the data are to be read from a data file, e.g. the test data file FIREBIRDSCE.FBDAT, then the DATA card must be replaced by the following card.

```
DATA(FILE=FIREBIRDSCE.FBDAT)
```

No data must be input after the ENTER command if the above card is used.

15. APPENDIX 8

Programs in SL's HELLFIRE suite of programs
(intended for use in connection with X-ray powder diffractometry

HELLFIRE1	EPIMETHEUS(14)	Validates experimental data
HELLFIRE2	FIRECRACKER(13)	Calibration
HELLFIRE2	FIRECRACKER2(15)	of X-ray
HELLFIRE2A	FIRECRACKER3(22)	diffractometers
HELLFIRE3A	FIRESTAR2(23)	Determination of lattice parameters.
HELLFIRE4	FIRERICE & FIRECHOP(24)	Rachinger separation of α_1 and α_2 Bragg reflections
HELLFIRE5	FIREBRAND(25)	Locates Bragg maximum
HELLFIRE6	FIREPLOT(26)	Plots out diffraction patterns and can smooth.
HELLFIRE7	FIREBIRD3(21)	Calculates the positions of Bragg reflections.
HELLFIRE8	FIREFLY3A (FIREBEE)(1)	Calculations of the
HELLFIRE8A	FIREFLY4(1)	intensities of Bragg
HELLFIRE8B	FIREFLY6 (FIRECOMET)20	reflections given the unit cell and if required the necessary Miller indices.
HELLFIRE9	FIREWOLF(27)	Integrates Bragg reflection intensity.
HELLFIRE10	FENRIS(28)	Derives crystallite sizes and strains from integral breadths.
HELLFIRE11	FAFNIR(29)	Derives crystallite sizes and strains from integral breadths, but includes possibility to calculate Scherrer constants for various types of prism.
HELLFIRE12	FIRENET(30)	Plots direct pole figures.

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